International Journal of Quantum Chemistry Author Index—Volume 60

Adams, W. H.
On the Limits of Validity of the Symmetrized Rayleigh–Schrödinger Perturabation Theory, 273
Ahsan, M. A. H. See Sarma, C. R., 147
Alfredsson, M.
—; Ojamäe, L.; Hermansson, K.: A comparison of Hartree–Fock, MP2, and DFT Results for the HCN Dimer and Crystal, 767
Alhambra, C. See Orozco, M., 1179
Allahverdiyev, S. I. See Guseinov, I. I., 637
Allan, N. L. See Measures, P. T., 579
Almlöf, J. See Røeggen, I., 453
Altmann, S. L.
Clifford Algebra, Symmetries, and Vectors, 359
Amos, A. T.
Bond Properties Using a Modern Version of the Drude Model, 67
Anderson, N.
—; Sutcliffe, B. T.: The Nuclear Motion Hamiltonian for a Tetratomic Molecule Considered as a Combination of an Atom and a Triatom, 37
Antipova, D. See Böhn, S., 649
Arrighini, G. P. See Lamanna, U. T., 475
Avery, J.
—; Hansen, T. B.: A Momentum-Space Picture of the Chemical Bond, 201
Azevedo, J. A. T. See Da Silva, C. O., 433

Bader, R. F. W.
—; Keith, T. A.: Use of Electron Charge and Current Distributions in the Determination of Atomic Contributions to Magnetic Properities, 373
Baeten, A.
—; De Proft, F.; Geerlings, P.: Proton Affinity of Amino Acids: Their Interpretation with Density Functional Theory-Based Descriptors, 931
Bała, P. See Grochowski, P., 1143
Balaban, A. T.
—; Klein, D. J.; Seitz, W. A.: Holes in Diamond or Carbon Nitride Lattices, 1065
Barandiarán, Z. See Seijo, L., 617
Barreiro, E. J. See De Sant'anna, C. M. R., 1069
Baxter, C. A.
—; Cook, D. B.: Molecular Fragments and the Hybrid Basis, 173
Bearpark, M. J.
—; Bernardi, F.; Olivucci, M.; Robb, M. A.: Potential Energy Surfaces of Pseudoaromatic Molecules: An MMVB and CASSCF Study of Pentalene, 505
Bergström, R.
Review of *Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy*, edited by S. R. Langhoff, 791
Bernardi, F. See Bearpark, M. J., 505
Berthier, G.
—; Defranceschi, M.; Tsoucaris, G.: Note on Origin-Shift Invariants and Phase Constraints for Momentum Space Wave Functions, 195
Bettega, M. H. F.
—; Natalense, A. P. P.; Lima, M. A. P.; Ferreira, L. G.: Note on the Generation of Gaussian Bases for Pseudopotential Calculations, 821
Bicca de Alencastro, R. See De Sant'anna, C. M. R., 1069
Bielińska-Wąż, D. See Karwowski, J., 185
Böhn, S.
—; Antipova, D.; Kuthan, J.: Study of Methanetriol Decomposition Mechanisms, 649
Brooks, B. R. See Eurenius, K. P., 1189
Busquets, M. A. See Orozco, M., 1179

Cacelli, I.
—; Moccia, R.: Differential Photoionization Cross Section Calculations for HI Using the Random-Phase Approximation with L^2 Basis Functions, 409
Cammi, R.
—; Cossi, M.; Mennucci, B.; Pomelli, C. S.; Tomasi, J.: Energy and Energy Derivatives for Molecular Solutes: Perspectives of Application to Hybrid Quantum and Molecular Methods, 1165
—; Tomasi, J.: Time-Dependent Variational Principle for Nonlinear Hamiltonians and Its Application to Molecules in the Liquid Phase, 297
Cartier, A.
—; Martins-Costa, M. T. C.; Rinaldi, D.: Computational of Electronic Molecular Polarizabilities by a Variational Method at the CISD Level, 883
Cassam-Chenaï, P.
—; Wolff, S. K.; Chandler, G. S.; Figgis, B. N.; Ensemble-Representable Densities for Atoms and Molecules. II Applications to $CoCl_4^{2-}$, 667
Chakrabarti, A.
—; Ramasesha, S.: Properties of

the Low-Lying Electronic States of Phenanthrene: Exact PPP Results, 381

Chandler, G. S. See Cassam-Chenaï, P., 667

Chatfield, D. C. See Eurenius, K. P., 1189

Chattaraj, P. K.

—; Ghosh, S. K.; Liu, S.; Parr, R. G.: Exchange–Correlation Potential and Excited-State Density Functional Theory, 535

Chaudhuri, R.

—; Datta, B.; Das, K.; Mukherjee, D.: A Spin-Adapted Coupled-Cluster Based Linear Response Theory for Double Ionization Potentials, 347

Chen, P. C.

Absorption Maxima Study of Chromophores of Indigoid Dyes, 681

Cimiraglia, R.

Many-Body Multireference Møller–Plesset and Epstein–Nesbet Perturbation Theory: Fast Evaluation of Second-Order Energy Contributions, 167

Colomines, C. See Orozco, M., 1179

Cook, D.

—; Sutcliffe, B.: Roy McWeeny, 1

Cook, D. B.

Virtual Orbitals, 793

—; See Baxter, C. A., 173

Cooper, D. L. See Cunningham, T. P., 393

—; See Karadakov, P. B., 545

—; See Measures, P. T., 579

—; See Raimondi, M., 225

Corma, A. See Planelles, J., 971

Cossi, M. See Cammi, R., 1165

Cundari, T. R.

—; Curtiss, S.: Substituent Effects on Methane Activation and Elimination by High-Valent Zr Complexes, 779

Cunningham, T. P.

—; Cooper, D. L.; Gerratt, J.; Karadakov, P. B.; Raimondi, M.: Chemical Bonding in Oxohalides of Hypercoordinate Nitrogen and Phosphorus, 393

Curtiss, S. See Cundari, T. R., 779

Dahl, J. P. See Schmider, H., 439

Dahl, T.

—; Skancke, P. N.: Structural Aspects of a Possible Transannular Interaction in Silatranes and Azasilatranes: An Ab Initio Study, 567

da Motta Neta, J. D. See De Sant'anna, C. M. R., 1069

Das, K. See Chaudhuri, R., 347

Da Silva, C. O.

—; Teixeira, F. E. C.; Azevedo, J. A. T.; Da Silva, E. C.; Nascimento, M. A. C.: Theoretical Characterization of the Ground State of the Alkaline-Earth Monocarbides: Ordering of the Two Lower-Lying States of the BeC, MgC, and CaC Molecules, 433

Da Silva, E. C. See Da Silva, C. O., 433

Datta, B. See Chaudhuri, R., 347

Datta, S. N.

—; Tandon, D.; Mallik, B.: Transfer of Excitation Energy in a Three-Dimensional-Doped Molecular Crystal. V. Self-Consistency of the Temporal Processes Involved in Energy Transfer in Photosynthetic Units, 1045

Day, O. W., Jr. See Morrison, R. C., 421

Deb, B. M. See Singh, H., 21

Defranceschi, M. See Berthier, G., 195

Dehareng, D. See Vancampenhout, N., 911

De Lara-Castells, M. P. See Gianturco, F. A., 593

Del Re, G.

Charge Transfer Between a Molecule and an Infinite Electron Reservoir in the MO Scheme, 141

De Proft, F. See Baeten, A., 931

de Sant'anna, C. M. R.

—; Bicca de Alencastro, R.; Fraga, C. A. M.; Barreiro, E. J.; da Motta Neto, J. D.: Molecular Modeling on Platelet-Activating Factor (PAF) and New Proposed PAF Antagonists, 1069

Deumens, E.

Review of Quaternionic Quantum Mechanics and Quantum Fields, by Stephen L. Adler, 941

de Vries, A. H. See van Duijnen, P. Th., 1111

Ding, F. J.

—; Zhang, L. F.: Gauche Effect and PM3 Calculation of Open-Chain Polyphosphorus Hydrides, 1037

Dive, G. See Vancampenhout, N., 911

Durante, N. See Lamanna, U. T., 475

Eurenius, K. P.

—; Chatfield, D. C.; Brooks, B. R.; Hodoscek, M.: Enzyme Mechanisms with Hybrid Quantum and Molecular Mechanical Potentials. I. Theoretical Considerations, 1189

Fabian, J. See Mann, M., 859

Fang, J.-Y.

—; Thomson, C.: Hydrogen-Bonding Effects, Electrostatic Potential, and the Antitumor Activity of Flavone Acetic Acid and Related Compounds. II Ab Initio Studies on the Second Stable Conformations, 897

Fernández-Serra, P. See Smeyers, Y. G., 493

Ferreira, L. G. See Bettega, M. H. F., 821

Field, M.

—; Gao, J.: Report for the Joint CECAM-NSF Planning Meeting on Hybrid Quantum and Classical Mechanical Methods for Simulation of Biopolymers in Solution (May 9–11, 1995), 1093

Figgis, B. N. See Cassam-Chenaï, P., 667

Fowler, P. W. See Steiner, E., 609

Fraga, C. A. M. See De Sant'anna, C. M. R., 1069
Friis-Jensen, B.
—; Rettrup, S.: Spin-Free Approach for Evaluation of Electronic Matrix Elements Using Character Operators of $\mathscr{S}_N$, 983
Fujimoto, H.
—; Sakata, K.; Fukui, K.: Transient Bonds and Chemical Reactivity of Molecules, 401
Fukui, K. See Fujimoto, H., 401

Gao, J. See Field, M., 1093
Garratt, J. See Karadakov, P. B., 545
Geerlings, P. See Baeten, A., 931
Gerratt, J. See Cunningham, T. P., 393
—; See Raimondi, M., 225
Ghosh, S. K. See Chattaraj, P. K., 535
Gianinetti, E.
—; Raimondi, M.; Tornaghi, E.: Modification of the Roothaan Equations to Exclude BSSE from Molecular Interaction Calculations, 157
Gianturco, F. A.
—; De Lara-Castells, M. P.: Stability and Structure of Rare-Gas Ionic Clusters Using Density Functional Methods: A Study of Helium Clusters, 593
Gineityte, V.
An Alternative Way of Solving Secular Equations for the Hamiltonian Matrices of Regular Quasi-One-Dimensional Systems, 717
Secular Polynomials for Chemical Graphs of Alkanes in Terms of Atoms and Bonds and Their Spectral Properties, 743
Golab, J. T. See Zakrzewski, V. G., 29
González-Guerra, A. See Smeyers, Y. G., 493
Grochowski, P.
—; Lesyng, B.; Bała, P.; McCammon, J. A.: Density Functional Based Parametrization of a Valence Bond Method and Its Applications in Quantum-Classical Molecular Dynamics Simulations of Enzymatic Reactions, 1143
Guidotti, C. See Lamanna, U. T., 475
Guo, X.
—; Randić, M.; Klein, D. J.: Analytical Expressions for the Count of LM-Conjugated Circuits of Benzenoid Hydrocarbons, 943
Guseinov, I. I.
—; İlík, A.; Allahverdiyev, S. I.: On the Evaluation of Overlap Integrals with the Same Screening Parameters of Slater-Type Orbitals Using Binomial Coefficients, 637

Hall, G. G. See Rees, D., 99
Hansen, T. B. See Avery, J., 201
Harcourt, R. D.
Increased-Valence Structures and Hypervalent Molecules, 553
Hermansson, K. See Alfredsson, M., 767
Heryadi, D. See Zakrzewski, V. G., 29
Hess, A. C. See Nada, R., 809
Hodoscek, M. See Eurenius, K. P., 1189
Huzinaga, S.
The Ab Initio Model Potential Method and the Optimized Orbitals for the Multiconfiguration Self-Consistent Field–Configuration Interaction Approach, 83

İlik, A. See Guseinov, I. I., 637

J. Dunne, L. J.
Review of *Dynamics During Spectroscopic Transitions—Basic Concept*, E. Lippert and J. D. Macomber, Eds., 709
Jaskolski, W. See Planelles, J., 971
—; See Rajadell, F., 993
Jaszuński, M.
—; Rizzo, A.: MCSCF Calculation of the Frequency-Dependent Hyperpolarizability of the Lithium Atom, 487
John P. E.
—; Mallion, R. B.: Calculating the Number of Spanning Trees in a Labeled Planar Molecular Graph Whose Inner Dual is a Tree, 59
Jug, K. See Ponec, R., 75
Jurkowski, J. See Karwowski, J., 185

Karadakov, P. B.
—; Garratt, J.; Cooper, D. L.; Raimondi, M.; Sironi, M.: Modern Valence-Bond Description of the Electronic Structure of Benzocyclobutadiene, 545
—; See Cunningham, T. P., 393
Karlsson, H. O.
Review of *Frontiers of Chemical Dynamics*, edited by E. Yurtsever, 789
Karwowski, J.
—; Bielińska-Wąż, D.; Jurkowski, J.: Eigenvalues of Model Hamiltonian Matrices from Spectral Density Distribution Moments: The Heisenberg Spin Hamiltonian, 185
Keith, T. A. See Bader, R. F. W., 373
Kikuchi, O. See Nakajima, H., 1081
Kinghorn, D. B. See Poshusta, R. D., 213
Klein, D. J. See Balaban, A. T., 1065
—; See Guo, X., 943
Kohout, M.
—; Savin, A.: Atomic Shell Structure and Electron Numbers, 875
Krause, J. L.
Review of *Ultrafast Processes in Chemistry and Photobiology*, M. A. El-Sayed, I. Tanaka, and Y. Molin, Eds., 713
Kryachko, E. S.
Lagrangian Many-Electron Molecular Dynamics—A Modern Tool for Attacking the Chemical Bond: The Physics Behind the Equations, 331
Kumar, A. See Mohan, C. G., 699
Kuthan, J. See Böhn, S., 649

Kutzelnigg, W.
—; Vogtner, S.: Extremal Electron Pairs, 235

Lamanna, U. T.
—; Durante, N.; Guidotti, C.; Arrighini; G. P.: Generalized Oscillator Strengths of Polyatomic Molecules. II. NH_3, 475
Lazzeretti, P.
—; Zanasi, R.: Molecular Magnetic Properties via Formal Annihilation of Paramagnetic Contribution to Electronic Current Density, 249
Lesyng, B. See Grochowski, P., 1143
Leszczyński, J. See Nowek, A., 1007
Li, X.
—; Paldus, J.: Bond Length Alternation in Cyclic Polyenes. VII. Valence Bond Theory Approch, 513
Lima, M. A. P. See Bettega, M. H. F., 821
Liu, S. See Chattaraj, P. K., 535
López, J. M. See Orozco, M., 1179
Luque, F. J. See Orozco, M., 1179
Luzzi, R. See Mesquita, M. V., 689

Maki, J.
—; Yamagishi, H.; Noro, T.; Sasaki, F.; Yamamoto, Y.: New "Localized Orbitals" Appropriate for Post-Hartree–Fock Calculations, 731
Mallik, B. See Datta, S. N., 1045
Mallion, R. B. See John, P. E., 59
Mann, M.
—; Fabian, J.: Ab Initio MO Calculations on 1,2-Dithietes and Valence Isomers, 859
March, N. H.
Momentum and Position Space Densities in Many-Electron Systems, 307
Martín-González, J. See Smeyers, Y. G., 493
Martins-Costa, M. T. C. See Cartier, A., 883

Matsubara, T.
—; Sieber, S.; Morokuma, K.: A Test of the New "Integrated MO + MM" (IMOMM) Method for the Conformational Energy of Ethane and *n*-Butane, 1101
McCammon, J. A. See Grochowski, P., 1143
McCarthy, M. I. See Nada, R., 809
McWeeny, R
Inside Story—Some Scientific Reminiscences, 3
Measures, P. T.
—; Allan, N. L.; Cooper, D. L.: Momentum–Space Electron Densities—Localized Orbitals in Hydrocarbons, Boranes, and Transition Metal Complexes, 579
Mennucci, B. See Cammi, R., 1165
Mesquita, M. V.
—; Vasconcellos, Á. R.; Luzzi, R.: Near-Dissipationless Coherent Excitations in Biosystems, 689
Micha, D. A.
Time-Evolution of Multiconguration Density Functions Driven by Nuclear Motions, 109
—; Review of *Statistical Mechanics and Thermodynamics*, Claude Garrod, 711
Ming, L.
Role of the Oxygen Content in $TlBa_{1.2}La_{0.8}CuO_{5+\delta}$ Superconductors, 1057
Mishra, P. C. See Mohan, C. G., 699
Moccia, R. See Cacelli, I., 409
Mohan, C. G.
—; Kumar, A.; Mishra, P. C.: An Optimized Approach to Compute Hybridization Displacement Charge and a Study of Its Effects on Electrostatic Potentials of Some Biologically Important Molecules, 699
Morokuma, K. See Matsubara, T., 1101
Morrison, R. C.
—; Tong, W.; Day, O. W., Jr.: Chemical Bonding in the Hydrogen Molecule, 421

Mukherjee, A. K. See Sarkar, J., 825
Mukherjee, D. See Chaudhuri, R., 347
Mukhopadhyay, A.
On a General System-Partitioning in the Many-Electron Correlation Problem, 261

Nada, R.
—; Nicholas, J. B.; McCarthy, M. I.; Hess, A. C.: Basis Sets for Ab Initio Periodic Hartree–Fock Studies of Zeolite/Adsorbate Interactions: He, Ne, and Ar in Silica Sodalite, 809
Nagaoka, M.
—; Yoshida, N.; Yamabe, T.: On the Equivalence Between the Microscopic Frictional Theory and Transition-State Theory, 287
Najjari, B. See Tavard, C., 657
Nakajima, H.
—; Kikuchi, O.: Analysis of Electrostatic and Hydrophobic Complementarities between Chymotrypsin and Avian Ovomucoid Third Domains Using Molecular Electrostatic Potential: Effect of Residue Replacements, 1081
Nascimento, M. A. C. See Da Silva, C. O., 433
Natalense, A. P. P. See Bettega, M. H. F., 821
Nicholas, J. B. See Nada, R., 809
Nichols, J. A. See Zakrzewski, V. G., 29
Nicolaides, C. A
The State-Specific Approach to the Solution of Problems of Electronic Structure and Dynamics Involving Excited States, 119
Nightingale, M. See Raynes, W. T., 529
Nordio, P. L.
—; Polimeno, A.: Classical Description of Activated Conformational Processes in Molecular Systems Coupled to Solvent Degrees of Freedom, 321
Noro, T. See Maki, J., 731

Nowek, A.
—; Leszczyński, J.: Post-Hartree–Fock and DFT Level Studies on the $Cl_2CO \cdots Cl_2$ Complex: Accurate Molecular Parameters, Harmonic Vibrational Frequencies, and Interaction Energies, 1007

Ojamäe, L. See Alfredsson, M., 767
Olivucci, M. See Bearpark, M. J., 505
Orozco, M.
—; López, J. M.; Colomines, C.; Alhambra, C.; Busquets, M. A.; Luque, F. J.: Theoretical Representation of Solvation in Biochemical Systems: From Discrete Solute–Solvent Interactions to Bulk Solvation, 1179
Ortiz, J. V. See Zakrzewski, V. G., 29

Paldus, J. See Li, X., 513
Palmieri, P. See Tarroni, R., 467
Parr, R. G. See Chattaraj, P. K., 535
Pauncz, R. See Rettrup, S., 91
Planelles, J.
—; Zicovich-Wilson, C.; Jaskolski, W.; Corma, A.: Semiempirical Hamiltonians for Spatially Confined π-Electron Systems, 971
—; See Rajadell, F., 993
Polimeno, A. See Nordio, P. L., 321
Pomelli, C. S. See Cammi, R., 1165
Ponec, R.
—; Jug, K.: Population Analysis of Pair Densities: A New Way of Visualization of Molecular Structure, 75
Poshusta, R. D.
—; Kinghorn, D. B.: Density Matrices for Correlated Gaussians: Helium and Dipositronium, 213
Pupyshev, V. I. See Scherbinin, A. V., 843

Raimondi, M.
—; Sironi, M.; Gerratt, J.; Cooper, D. L.: Optimized Spin-Coupled Virtual Orbitals, 225
—; See Cunningham, T. P., 393
—; See Gianinetti, E., 157
—; See Karadakov, P. B., 545
Rajadell, F.
—; Planelles, J.; Jaskolski, W.; Zicovich-Wilson, C.: Selection of Basis Sets for Atoms and Molecules in Cavities, 993
Ramasesha, S. See Chakrabarti, A., 381
Randić, M. See Guo, X., 943
Raynes, W. T.
—; Nightingale, M.: Calculation of ^{13}C Shielding of the Isotopomers CH_3Cl, CH_2DCl, CHD_2Cl, and CD_3Cl, 529
Rees, D.
—; Hall, G. G.: Localized Functions of a Sphere, 99
Rettrup, S.
—; Pauncz, R.: Representations of the Symmetric Group Generated by Projected Spin Functions: A Graphical Approach, 91
—; See Friis-Jensen, B., 983
Rinaldi, D. See Cartier, A., 883
Rizzo, A. See Jaszuński, M., 487
Robb, M. A. See Bearpark, M. J., 505
Røeggen, I.
—; Almlöf, J.: Interatomic Potential for the $X^1\Sigma_g^+$ State of Be_2, 453
Rosmus, P. See Tarroni, R., 467
Rothstein, S. M.
Valence Energy in Variational Monte Carlo: CuH Dissociation Energy, 803
Ruette, F. See Sierraalta, A., 1015

Sagan, B. E.
—; Yeh, Y.-N.; Zhang, P.: The Wiener Polynomial of a Graph, 959
Sakata, K. See Fujimoto, H., 401
Sarkar, J.
—; Mukherjee, A. K.: Factorization of Interaction Graphs with n-fold Symmetry: Some Applications in PPP Calculation and Molecular Vibrational Analysis, 825
Sarma, C. R.
—; Ahsan, M. A. H.: Electron Correlation Studies: Rumer Basis Approach, 147
Sasaki, F. See Maki, J., 731
Savin, A. See Kohout, M., 875
Scherbinin, A. V.
—; Pupyshev, V. I.; Stepanov, N. F.: On the Use of Multipole Expansion of the Coulomb Potential in Quantum Chemistry, 843
Schmider, H.
—; Dahl, J. P.: Nodal Structure of the Electronic Wigner Function of Many-Electron Atoms and Molecules, 439
Schreckenbach, G.
—; Ziegler, T.: The Calculation of NMR Shielding Tensors Based on Density Functional Theory and the Frozen-Core Approximation, 753
Seijo, L.
—; Barandiarán, Z.: Applications of the Group-Function Theory to the Field to Materials Science, 617
Seitz, W. A. See Balaban, A. T., 1065
Sieber, S. See Matsubara, T., 1101
Sierraalta, A.
—; Ruette, F.: The Laplacian of the Electronic Density at the Valence-Shell Charge Concentration (VSCC): A Comparative Study of Effective Core Potential and Full-Electron Calculations in Mo Compounds. II, 1015
Singh, H.
—; Sukumar, N.; Deb, B. M.: "Atom" as a Complex System: One- and Two-Dimensional Cellular Automata Simulations, 21
Sironi, M. See Karadakov, P. B., 545
—; See Raimondi, M., 225
Skanchke, P. N. See Dahl, T., 567
Smeyers, Y. G.
—; González-Guerra, A.; Martín-González, J.; Fernández-Serra, P.: A Study of the Molecular Orbital Localization into an Extended Hartree–Fock Ap-

proach: Application to the BeH_2 Ground State, 493
Steiner, E.
—; Fowler, P. W.: Ring Currents in Aromatic Hydrocarbons, 609
Stepanov, N. F. See Scherbinin, A. V., 843
Suffczyński, M. See Ungier, W., 1001
Sukumar, N. See Singh, H., 21
Sutcliffe, B. See Cook D., 1
Sutcliffe, B. T. See Anderson, N., 37

Tandon, D. See Datta, S. N., 1045
Tarroni, R.
—; Palmieri, P.; Rosmus, P.: On the Lowest Electronic States of the C_2F Radical, 467
Taşeli, H.
Accurate Lower and Upper Bounds of the Energy Spectrum for the Asymmetrical Two-Well Potentials, 641
Tavard, C.
—; Najjari, B.: Importance of Angular and Radial Electron Correlations in First Born (e, $2e$) Spectroscopies of Helium-like Targets, 657
Teixeira, F. E. C. See Da Silva, C. O., 433
Thompson, M. A.
Molecular Dynamics Study of a New Rigidified 18-Crown-6 Derivative Using a QM/MM Method, 1133
Thomson, C. See Fang, J.-Y., 897
Tomasi, J. See Cammi, R., 297, 1165
Tong, W. See Morrison, R. C., 421
Tornaghi, E. See Gianinetti, E., 157
Tsoucaris, G. See Berthier, G., 195

Ungier, W.
—; Suffczyński, M.: A Simple Method of Treating Integrals Containing Hylleraas–Ore Molecular Functions, 1001

Valdemoro, C.
Contracting and Calculating Traces Over the N-Electron Space: Two Powerful Tools for Obtaining Averages, 131
Vancampenhout, N.
—; Dive, G.; Dehareng, D.: Energetic and Conformational Study of Four Benzylimidazole Compounds with $\alpha 2$ Agonist Profile: The Mivazerol and Three Methylated Derivatives, 911
van Duijnen, P. Th.
—; de Vries, A. H.: Direct Reaction Field Force Field: A Consistent Way to Connect and Combine Quantum-Chemical and Classical Descriptions of Molecules, 1111
Vasconcellos, Á. R. See Mesquita, M. V., 689
Vogtner, S. See Kutzelnigg, W., 235

Wang, Y.-G. See Zong, S.-J., 833
Wasilewski, J.
—; Zelek, S.; Wierzbowska, M.: Modifications of Virtual Orbitals in the Limited CI Calculations for Electron-Rich Molecules, 1027
Wierzbowska, M. See Wasilewski, J., 1027
Wilson, S.
Distributed Basis Sets of s-Type Gaussian Functions for Molecular Electronic Structure Calculations: Applications of the Gaussian Cell Model to One-Electron Polycentric Linear Molecular Systems, 47
Wolff, S. K. See Cassam-Chenaï, P., 667

Xu, W.-X.
Parallel Electron Correlation Effect and Fermi Hole Structure, 853

Yamabe, T. See Nagaoka, M., 287
Yamagishi, H. See Maki, J., 731
Yamamoto, Y. See Maki, J., 731
Yeager, D. L. See Zakrzewski, V. G., 29
Yeh, Y.-N. See Sagan, B. E., 959
Yoshida, N. See Nagaoka, M., 287

Zakrzewski, V. G.
—; Ortiz, J. V.; Nichols, J. A.; Heryadi, D.; Yeager, D. L.; Golab, J. T.: Comparison of Perturbation and Multiconfigurational Electron Propagator Methods, 29
Zanasi, R. See Lazzeretti, P., 249
Zang, Q.-E. See Zong, S.-J., 833
Zelek, S. See Wasilewski, J., 1027
Zhang, L. F. See Ding, F. J., 1037
Zhang, P. See Sagan, B. E., 959
Zhong, S.-J.
—; Wang, Y.-G.; Zhang, Q.-E.: Symmetry Reduction of the Matrix Elements of Two-Particle Operator, 833
Zicovich-Wilson, C. See Planelles, J., 971
—; See Rajadell, F., 993
Ziegler, T. See Schreckenbach, G., 753

International Journal of Quantum Chemistry Subject Index—Volume 60

Ab initio, 567, 617, 649, 681, 897, 911
Ab initio calculations, 173, 1037
Ab initio full-electron (FE) calculations, 1015
Ab initio MO calculations, 859
Ab initio model potential method, 83
Ab initio periodic Hartree–Fock (PHF) calculations, 809
Ab initio post-Hartree–Fock theory, 1007
Ab initio quantum-chemical descriptions of matter, 1111
Ab initio wave functions, 75
Absorption maxima, 681
Adiabatic energy surfaces, 467
Alkaline-earth element, 433
Alkanes, 743
All-electron approach, 803
α2 adrenoceptors, 911
Amono acids, 931
Angular electron correlations, 657
Antitumor activity, 897
Approximate valence bond (AVB) method, 1143
Asymmetrical two-well oscillators, 641
Atomic hybrids, 99
Atomic natural orbitals (ANO), 467
Atomic shell structure, 875
Auger spectroscopy, 347
Average, 131
Azasilatranes, 567

Basis-set atomic orbitals (AO), 331
Basis set superposition error (BSSE), 157
Basis sets, 47, 201, 809, 993
Benzenoid hydrocarbons, 943
Bethe surface, 475
Binding energy, 453
Bionomial coefficients, 637
Biosystems, 689
Bond length alternation, 513
Bond properties, 67
Bonding patterns, 75

CASSCF calculations, 505
C coefficients, 833
Cellular automata (CA) simulations, 21
Charge transfer, 141
Chebyshev polynomials, 743
Chromophores, 681
CISD level, 883
Clifford algebra, 359
Complementarities, 1081
Complete-active-space self-consistent field (CAS SCF) approach, 545
Configuration interaction (CI), 593
Configuration interaction (CI) calculations, 433, 1027
Configuration interaction (CI) coefficients, 331
Configuration interaction (CI) methods, 983
Configuration state functions (CSF), 147
Coordinative bonds, 1065
Core–valence partitioning scheme, 803
Correlated Gaussian basis functions, 213
Correlation charge, 853
Coulomb potential, 843
Couple-ionization potentials (DIPs), 347
Coupled-cluster based linear response theory (CC-LRT), 347
Coupled Hartree–Fock theory, 609
Covalent bonding, 393
Cross-section calculations, 821
Cuboidal cavities, 993
Current distributions, 373

Davydov solitons, 689
Density functional theory (DFT), 767
Density functional theory (DFT), 593, 931, 1007
Density matrices, 109, 213, 731
Diamond-lattice-based structures, 1065
Diffusion-only Metroplis algorithm, 803
Direct reaction field (DRF) force field, 1111
d-orbital participation, 393
Drude model, 67

Effective core potential (ECP), 1015
Eigenvalues, 185
Electric dipole hyperpolarizability, 487
Electron charge, 373
Electron correlation, 235
Electron delocalization, 401
Electron density, 21, 421
Electron localization function (ELF), 875
Electron propagator techniques, 29
Electron reservoir, 141
Electronic configuration, 821
Electronic matrix elements, 983
Electronic polarizabilities, 883
Electronic structure, 119
Electrostatic, 1081
Electrostatic potential maps, 699
Energy transfer, 1045
Ensemble density, 667
Enzymatic reactions, 1143
Enzymes, 1189
Epstein–Nesbet perturbation theory, 167
Euclidean-group operations, 359
Exchange correlation energy, 853
Exchange–correlation potential, 535
Excited-state density functional theory, 535
Exponents, 331

External electromagnetic fields, 119
External magnetic field, 609
Extremal electron pairs, 235

Fermi hole, 853
Fock's solutions, 201
Formal annihilation, 249
Four-particle system 1001
Fragments, 173
Fröhlich's effect, 689
Frozen-core approximation, 753
Functional theory (DFT), 753

Gaussian bases, 821
Gaussian cell model, 47
Generalized oscillator strengths, 475
Generalized overlap amplitudes, 421
Generalized valence bond (GVB), 433
Gibbs vectors, 359
Graphs, 959
Group-function theory, 617

Hamiltonian, 37
Hamiltonian matrices, 717
Hamiltonians, 185, 297, 971
Hartree–Fock, 767
Hartree–Fock approach, 493
Hartree–Fock multiconfiguration self-consistent field (HF–MCSCF) ab initio method, 467
HCN Dimer, 767
Heisenberg spin Hamiltonian spectrum, 185
Helium ionic clusters, 593
High-valent zirconium complexes, 779
Holes, 1065
Hybrid atomic orbital basis, 173
Hybrid quantum mechanical and molecular mechanical (QM/MM) potentials, 1189
Hybridization displacement charge (HDC), 699
Hydrocarbons, 609
Hydrogen-bonding effects, 897
Hydrophobic complementarities, 1081
Hylleraas–Ore wave functions, 1001
Hyperpolarizability, 487
Hypervalent molecules, 553

Increased-valence structures, 553
Indigoid dyes, 681
Informational statistical thermodynamics, 689
Interatomic potential, 453
Intermolecular interaction energies, 273
Intermolecular interactions, 1111
Intregrated molecular orbital + molecular mechanics (IMOMM) method, 1101
Inverted order of operations, 717
Ionization energies, 29
Isotopomers, 529

Kekulé structures, 943

La-doped superconductors, 1057
Lagrangian many-electron molecular dynamics, 331
Linear extended π-electron systems, 513
LM-conjugated circuits, 943
Löwdin charge distributions, 699
Low-lying electronic states, 381
Lower-lying electronic states, 433
Lowest electronic states, 467
L^2 basis set calculation, 409

Magnetic response properties, 373
Magnetic susceptibilities, 249
Magnetization, 667
Many-electron atoms, 439
Many-electron correlation problem, 261
Many-electron molecules, 439
Many-electron systems, 147, 307
Materials science, 617
Medium-size polarized (MSPBS) basis sets, 1007
Metal complexes, 579
Methane activation, 779
Methane elimination, 779
Methanetroil decomposition mechanisms, 649
Microscopic frictional theory, 287
Møller–Plesset perturbation theory, 167
Model Hamiltonian matrices, 185
Modern valence bond (VB) theory, 545
Modified virtual orbitals (MVO), 1027
Molecular dynamics (MD), 1133
Molecular electrostatic potential (MEP), 897, 1081
Molecular graph, 59
Molecular interactions, 157
Molecular matrix elements, 833
Molecular modeling, 1069
Molecular orbitals, 579
Molecular orbitals (MO), 141
Molecular orbitals (MOs), 493, 793
Molecular vibration, 825
Momentum–space electron densities, 579
Momentum space moments, 307
Momentum space quantum chemistry, 195
Monte Carlo method, 803
MP2, 767
Mulliken charge distributions, 699
Multicenter bonding, 75
Multiconfiguration SCF wave functions, 487
Multiconfiguration self-consistent field–configuration interaction (MCSCF–CI), 83
Multiconfiguration time-dependent Hartree–Fock (MC-TDHF) approach, 109
Multipole expansion, 843

n-electron wave function, 235
N-electron space, 131
n-fold symmetry, 825
Nonlinear Hamiltonians, 297
Nuclear magnetic resonance (NMR) spectroscopy, 753
Nuclear motion Hamiltonian, 37
Nuclear motions, 109

Onsager's solvent model, 911
Open-chain phosphoanes, 1037
Optimized equilibrium, 1101
Optimized orbitals, 83
Orbitals, 793
Origin-shift invariants, 195
Orthogonalized natural orbitals (ONO), 1027
Overlap integrals, 637
Oxygen content, 1057

Pair densities, 75
Parallel electron correlation coefficient, 853
Paramagnetic contribution, 249

Pariser–Parr–Pople (PPP) calculations, 825
Pariser–Parr–Pople (PPP) model, 381
Perturbation theory (PT), 167
Perturbative formalism, 29
Phase invariance, 195
Photonionization cross sections, 409
Photosynthetic units, 1045
π-electron systems, 971
Platelet-activating factor (PAF), 1069
PM3 method, 1037
Polar solvents, 321
Polarizable continuum model (PCM), 1165
Polyatomic systems, 493
Polycentric molecule, 47
Post-Hartree–Fock calculations, 731
Potential energy surfaces, 505
Projected spin functions, 91
Proton affinity, 931
Pseudoaromatic molecules, 505
Pseudopotentials, 821

Quantum mechanical current density, 249
Quantum-classical molecular dynamics (QCMD) simulations, 1143
QM/MM Method, 1133

Radial electron correlations, 657
Random-phase approximation (RPA), 409
Random-phase approximation approach, 475
Rayleigh–Ritz variational method, 641
Reactive dynamics, 321
Reciprocal-space Schrödinger equation, 201
Regular quasi-one-dimensional systems, 717
Representation matrices, 91
Restricted Hartree–Fock (RHF), 433
Rigidfied 18-crown-6 derivative, 1133
Roothaan equations, 157
Rumer spin-coupling scheme, 147

Schrodinger equation, 641
Secular polynomials, 743
Self-consistent field (SCF), 75, 529
Self-consistent group formalism, 173
Semiemperical π-Hamiltonians, 971
Silatranes, 567
Singlet transitions, 475
Slater-type orbitals, 637
Solute–solvent interactions, 1179
Solute–solvent potential, 1165
Solute, 321
Solutes, 1165, 1179
Solvation, 1165
Solvent degrees of freedom, 321
Solvents, 1179
Spanning trees, 59
Spectral density distribution moments, 185
Sphere, 99
Spherical cavities, 993
Spin-independent many-electron Hamiltonian, 983
Spinshift formalism, 261
State-specific approach (SSA), 119
Sturmain basis sets, 201
Subsystems, 731
Symmetrized Rayleigh–Schrödinger (SRS) perturbation theory, 273
Symmetry operations, 833

^{13}C shielding, 529
Three-dimensional-doped molecular crystal, 1045
Transannular internuclear distances, 567
Transient bonds, 401
Transition-metal (TM) complexes, 779
Transition-state theory, 287
Transition states, 649
Transition structures, 1101
Triatomic, 37
Trigonometric basis sets, 641
Two-sided eigenvalue bounds, 641

Valence bond (VB) wave functions, 225
Valence bond theory, 513
Valence energies, 803
Valence isomerization, 859
Valance-shell charge concentration (VSCC), 1015
Variational Method, 883
Variational wave functions, 297
Virtual orbitals, 225, 793

Wave functions, 657
Weiner polynomial, 959
Wiener index, 959
Wigner function, 439